

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.63

Global applicability domain: Inside

Local applicability domain index: 4.11e-01

Confidence level: 6.07e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Oxydisulfoton</div> <div>Measured: 1.00</div> <div>Predicted: 1.63</div>	<div>Image not found</div> <div>Disulfoton sulfone</div> <div>Measured: 5.01</div> <div>Predicted: 3.83</div>	<div>Image not found</div> <div>lprobenfos</div> <div>Measured: 8.71</div> <div>Predicted: 4.13</div>
<div>Image not found</div> <div>Disulfoton</div> <div>Measured: 219</div> <div>Predicted: 151</div>	<div>Image not found</div> <div>Mesulfenfos</div> <div>Measured: 1.32</div> <div>Predicted: 1.62</div>	